PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 11, March 04, 2021 (Thursday)

- Reading:
  Postulates of Quantum Mechanics and Schrödinger Equation
  [Griffiths 1 and 2]
- Assignment: Problem Set 5 due March 05 (Friday).
  Submit your homework assignments to Canvas.

Topics for Today: Postulates of Quantum Mechanics

3.4 The Uncertainty Principle

3.5 Ehrenfest's Theorem

Topics for Next Lecture:
Schrödinger Equation [Griffiths 1 and 2]

3.6 Stationary State Solutions

3.7 Schrödinger Equation

(a) Infinite Square Well

(b) Finite Square Well.

(c) The Delta-Function Potential

3.8 Equation of continuity

3.4 The Uncertainty Principle

Let A and B be two non-commuting operators with

$$[A, B] = i\hbar$$

As we have seen before, these are conjugate operators. Let ΔA be the root mean square deviation of the operator A. Thus

$$(\Delta A)^2 \quad \equiv \quad \langle A^2 \rangle - \langle A \rangle^2$$

Similarly let ΔB be the root mean square deviation of the operator B. Thus

$$(\Delta B)^2 = \langle B^2 \rangle - \langle B \rangle^2$$

then

$$\Delta A \Delta B \geq \frac{\hbar}{2} \;\; \mathrm{(Heisenberg's \;\; uncertainty \;\; principle)}$$

First of all notice that

$$
\begin{aligned}
(\Delta\Omega)^2 &= \langle\Omega^2\rangle - \langle\Omega\rangle^2 \\
&= \langle\Omega^2 - 2\Omega\langle\Omega\rangle + \langle\Omega\rangle^2\rangle \\
&= \langle(\Omega - \langle\Omega\rangle)^2\rangle \\
\Delta\Omega &\equiv \langle(\Omega - \langle\Omega\rangle)^2\rangle^{1/2} \; = \; \left[\Omega^2\rangle - \langle\Omega\rangle^2\right]^{1/2}
\end{aligned}
$$

where (i) $\Delta\Omega$ is the standard deviation which measures the average fluctuation around the mean.

N.B. (i) $\Delta\Omega$ is often called the root mean squared deviation or the uncertainty in Ω.
(ii) $(\Delta\Omega)^2$ is called the mean square deviation or the variance.

Let us define

$$\delta A \equiv A - \langle A \rangle \quad \text{and} \quad \delta B \equiv B - \langle B \rangle.$$

Then we have $[\delta A, \delta B] = [A, B] = i\hbar$. Furthermore,

$$\begin{aligned}
(\Delta A)^2 (\Delta B)^2 &= \langle (A - \langle A \rangle)^2 \rangle \langle (B - \langle B \rangle)^2 \rangle \\
&= \langle (\delta A)^2 \rangle \langle (\delta B)^2 \rangle \\
&\geq |\langle \delta A \delta B \rangle|^2 \ \ \text{(Schwartz inequality)} \\
&= |\langle \frac{1}{2}(\delta A \delta B + \delta B \delta A) + \frac{1}{2}(\delta A \delta B - \delta B \delta A) \rangle|^2 \\
&= |\langle \frac{1}{2}(\delta A \delta B + \delta B \delta A) + \frac{1}{2}[\delta A, \delta B] \rangle|^2 \\
&= |\langle \frac{1}{2}(\delta A \delta B + \delta B \delta A) + \frac{1}{2}(i\hbar) \rangle|^2 \quad \text{(complex } z = x + iy\text{)} \\
&= |\langle \frac{1}{2}(\delta A \delta B + \delta B \delta A) \rangle|^2 + \frac{\hbar^2}{4} \qquad (|z|^2 = x^2 + y^2)\,.
\end{aligned}$$

Therefore,

$$\Delta A \Delta B \geq \frac{\hbar}{2}.$$

- This tells us that for any two conjugate variables, there is a minimum of uncertainty associated with their measurements.
- Note that the Schwartz inequality becomes an equality if the vectors are parallel to each other. Thus

$$\delta A|\psi\rangle = \lambda \delta B|\psi\rangle$$

and

$$\begin{aligned}
\frac{1}{2}\langle\psi|(\delta A\delta B + \delta B\delta A)|\psi\rangle &= \frac{1}{2}\langle\psi|\lambda^*\delta B\delta B + \lambda\delta B\delta B)|\psi\rangle \\
&= \frac{1}{2}(\lambda^* + \lambda)\langle\psi|\delta B\delta B|\psi\rangle \\
&= \frac{1}{2}(\lambda^* + \lambda)\langle\delta B\psi|\delta B\psi\rangle\,.
\end{aligned}$$

If this vanishes, then we have

$$(\Delta A)(\Delta B) = \frac{\hbar}{2}$$

which is the minimum uncertainty.

Now we have

$$\frac{1}{2}\langle\psi|(\delta A\delta B + \delta B\delta A)|\psi\rangle = 0 \quad \text{if} \quad \frac{1}{2}(\lambda^* + \lambda)\langle\delta B\psi|\delta B\psi\rangle = 0\,.$$

Since $\langle\delta B\psi|\delta B\psi\rangle$ is greater than zero unless $|\delta B\psi\rangle = 0$, then

$$\lambda^* + \lambda = 0 \quad \text{or} \quad \lambda^* = -\lambda\,.$$

Thus λ is pure imaginary.

Let $\lambda = -ic$ where c is real. Then we have

$$\delta A|\psi\rangle = \lambda\delta B|\psi\rangle = -ic\delta B|\psi\rangle.$$

N.B. $\langle\Omega\rangle = \langle\psi|\Omega|\psi\rangle$ and $|\Omega\psi\rangle \equiv \Omega|\psi\rangle$.

Furthermore, we know that

$$\delta A = A - \langle A \rangle \quad \text{and} \quad \delta B = B - \langle B \rangle \,.$$

Since A and B are conjugate operators, we can express them as differential operators. For example

$$\langle x|P|y\rangle = -i\hbar \frac{d}{dx}\delta(x-y) \text{ (x basis)} \;\text{ and }\; \langle p|X|q\rangle = i\hbar \frac{d}{dp}\delta(p-q) \text{ (p basis)}.$$

In the x basis, let us consider

$$A = X \,, \qquad B = P \to -i\hbar \frac{d}{dx} \,, \quad \text{and} \quad \delta X|\psi\rangle = \lambda \delta P|\psi\rangle = -ic\delta P|\psi\rangle \,.$$

Then we have

$$(x - \langle X\rangle)\,\psi(x) = -ic\left(-i\hbar\frac{d}{dx} - \langle P\rangle\right)\psi(x)$$

or

$$\frac{d\psi}{dx} = -\frac{1}{c\hbar}\,(x - \langle X\rangle - ic\langle P\rangle)\,\psi(x)$$

and then

$$\psi(x) = N \exp\left[-\frac{1}{2c\hbar}(x - \langle X \rangle)^2 + \frac{i}{\hbar}\langle P \rangle x\right].$$

This is a Gaussian centered at $x = \langle X \rangle$ with a width Δx given by

$$\frac{1}{(\Delta x)^2} = \frac{1}{c\hbar}$$

where N is the normalization constant.

Exercise: Find the normalization constant for

$$\psi(x) = N \exp\left[-\frac{1}{2c\hbar}(x - \langle X \rangle)^2 + \frac{i}{\hbar}\langle P \rangle x\right]$$

such that

$$\int |\psi(x)|^2 \, dx = 1.$$

3.5 Ehrenfest's Theorem

Let us consider an operator Ω and its expectation value $\langle\Omega\rangle \equiv \langle\psi|\Omega|\psi\rangle$ in a state with state vector $|\psi\rangle$.

We are interested in the change of $\langle\Omega\rangle$ in time

$$\begin{aligned}\frac{d}{dt}\langle\Omega\rangle &= \frac{d}{dt}\langle\psi|\Omega|\psi\rangle \\ &= \langle\dot{\psi}|\Omega|\psi\rangle + \langle\psi|\frac{\partial}{\partial t}\Omega|\psi\rangle + \langle\psi|\Omega|\dot{\psi}\rangle\,.\end{aligned}$$

We know from Schrödinger equation that

$$\begin{aligned}i\hbar\frac{d}{dt}|\psi\rangle &= i\hbar|\dot{\psi}\rangle \;=\; H|\psi\rangle \\ -i\hbar\langle\dot{\psi}| &= \langle\psi|H\,.\end{aligned}$$

N.B. The Hamiltonian is Hermitian $H^\dagger = H$.

Substituting this into the above equation we have

$$\begin{aligned}\frac{d}{dt}\langle\Omega\rangle &= \langle\dot{\psi}|\Omega|\psi\rangle + \langle\psi|\frac{\partial}{\partial t}\Omega|\psi\rangle + \langle\psi|\Omega|\dot{\psi}\rangle \\ &= \frac{i}{\hbar}\langle\psi|H\Omega|\psi\rangle + \langle\psi|\frac{\partial}{\partial t}\Omega|\psi\rangle - \frac{i}{\hbar}\langle\psi|\Omega H|\psi\rangle \\ &= \langle\psi|\frac{\partial}{\partial t}\Omega|\psi\rangle - \frac{i}{\hbar}\langle\psi|[\Omega, H]|\psi\rangle\,.\end{aligned}$$

If the operator Ω has no explicit time dependence, then we can write

$$\frac{d}{dt}\langle\Omega\rangle = -\frac{i}{\hbar}\langle\psi|[\Omega, H]|\psi\rangle \quad \text{or} \quad i\hbar\frac{d}{dt}\langle\Omega\rangle = \langle\psi|[\Omega, H]|\psi\rangle\,.$$

This is known as Ehrenfest's Theorem.

We now have

$$\frac{d\Omega}{dt} = -\frac{i}{\hbar}[\Omega, H] \quad \text{similar to} \quad \frac{d\omega}{dt} = \{\omega, H\}$$

which is Hamilton's equation of motion.

The quantum correspondence principle is expressed as

$$[\Omega_1, \Omega_2] = i\hbar\{\omega_1, \omega_2\} = i\hbar \sum_i \left(\frac{\partial \omega_1}{\partial x_i}\frac{\partial \omega_2}{\partial p_i} - \frac{\partial \omega_1}{\partial p_i}\frac{\partial \omega_2}{\partial x_i} \right) .$$

We can consider

$$\langle [\Omega, H] \rangle = i\hbar \langle \{\omega, H\} \rangle = i\hbar \frac{d}{dt}(\omega) = i\hbar \frac{d}{dt}\langle \Omega \rangle$$

that is

$$i\hbar \frac{d}{dt}\langle \Omega \rangle = \langle [\Omega, H] \rangle .$$

Example:

Let us consider the motion of one particle with

$$H = \frac{P^2}{2m} + V(X) \to H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\,.$$

We can investigate

$$\begin{aligned}
\frac{d\langle X\rangle}{dt} &= \frac{d}{dt}\langle\psi|X|\psi\rangle \\
&= -\frac{i}{\hbar}\langle\psi|[X,H]|\psi\rangle \\
&= -\frac{i}{\hbar}\langle\psi|[X,\frac{P^2}{2m}+V(x)]|\psi\rangle \\
&= -\frac{i}{\hbar}\langle\psi|[X,\frac{P^2}{2m}]|\psi\rangle \\
&= -\frac{i}{\hbar}\frac{1}{2m}\langle\psi|P[X,P]+[X,P]P|\psi\rangle \\
&= -\frac{i}{\hbar}\frac{1}{2m}(2i\hbar)\langle\psi|P|\psi\rangle \;=\; \frac{1}{m}\langle\psi|P|\psi\rangle\,.
\end{aligned}$$

We have found

$$\frac{d}{dt}\langle X\rangle = -\frac{i}{\hbar}\langle\psi|[X,H]|\psi\rangle = \frac{\langle P\rangle}{m}\,.$$

In classical mechanics, we know that

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}\,, \quad \text{and} \quad \dot{p} = -\frac{\partial H}{\partial x} = -\frac{d}{dx}V(x)\,.$$

Thus we have seen that for an operator Ω, the expectation value $\langle\Omega\rangle$ has the following evolution equation

$$\frac{d}{dt}\langle\Omega\rangle = -\frac{i}{\hbar}\langle[\Omega,H]\rangle$$

or

$$i\hbar\frac{d}{dt}\langle\Omega\rangle = \langle[\Omega,H]\rangle\,.$$

That means the expectation value of an operator $\langle\Omega\rangle$ follows the classical equation of motion.

Let us consider a system with the state vector $|\psi\rangle$.

- The position measurement yields a value x with uncertainty ΔX.
- And the momentum measurement yields a value p with uncertainty

$$\Delta P \simeq \frac{\hbar}{2\Delta X}\,.$$

Note that the uncertainty relation for X and P is

$$\Delta X \Delta P \geq \frac{\hbar}{2}\,.$$

If the state is such that the uncertainties ΔX and ΔP are negligible compared to the measured values x and p then we replace

$$\langle X \rangle = x \quad \text{and} \quad \langle P \rangle = p$$

where x and p are classical quantities.

For such a state, therefore, the fluctuation around the mean is negligible and we can write

$$\langle \Omega(X,P) \rangle = \Omega(\langle X \rangle, \langle P \rangle) = \Omega(x,p) = \omega(x,p)$$

Therefore in such a case we can write the Ehrenfest equation as

$$\frac{d}{dt}\langle \Omega \rangle = \frac{d\omega}{dt} = \{\omega, H\}$$

which is Hamilton's equation.

Thus we see that quantum mechanics reduces to classical Hamiltonian mechanics when it is applied to macroscopic systems.